

Calculations of Nuclear Astrophysics and Californium Fission Neutron Spectrum Averaged Cross Section Uncertainties using ENDF/B-VII.1, JEFF-3.1.2, JENDL-4.0 and Low-Fidelity Covariances

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Nuclear astrophysics and californium fission neutron spectrum averaged cross sections and their uncertainties for ENDF materials have been calculated. Absolute values were deduced with Maxwellian and Mannhart spectra, while uncertainties are based on ENDF/B-VII.1, JEFF-3.1.2, JENDL-4.0 and Low-Fidelity covariances. These quantities are compared with available data, independent benchmarks, EXFOR library, and analyzed for a wide range of cases. Recommendations for neutron cross section covariances are given and implications are discussed.

I. INTRODUCTION

Calculations of integral values at NNDC have been conducted in parallel with the ENDF/B-VII library releases [1, 2]. These values represent the complementary data sets for nuclear astrophysics, industry, and data evaluation applications. First results on reaction rates and neutron cross sections [3] have demonstrated a large potential of ENDF/B-VII for applications, such as KADoNiS stellar nucleosynthesis library [4]. Further interactions with the fundamental and applied science communities have initiated work on the extended list of integral values and their uncertainties [5–7]. Calculations of nuclear astrophysics and californium fission neutron spectrum averaged cross section (*i.e.* californium spectrum) uncertainties are presented in the following sections.

II. MAXWELLIAN-AVERAGED CROSS SECTIONS UNCERTAINTIES

Nuclear data covariances are essential for fundamental and applied nuclear science and technology. They provide the experimentally-observable uncertainties that are necessary for application development. Maxwellian-averaged cross sections and their uncertainties have been calculated in recent years [3, 5]. Fig. 1 shows cross section uncertainties for ENDF/B-VII.1 evaluated library, Low Fidelity project, and KADoNiS database [2, 4, 8] demonstrate nuclear astrophysics value of ENDF and Low Fidelity covariances for stellar nucleosynthesis research. At

the same time, the ENDF/B-VII.1 and Low Fidelity uncertainties are relatively large for precise calculations. The stellar nucleosynthesis calculations require the stringent cross section uncertainties in order $<3\%$ to finalize the branching of the *s*-process path. However, even a specially-designated KADoNiS library, at the present state, cannot satisfy this requirement, and further research is necessary.

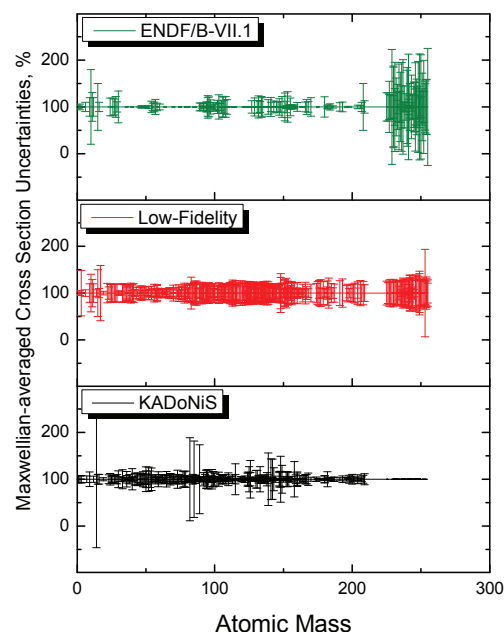


FIG. 1. (Color online) Maxwellian-averaged neutron capture cross section, $kT=30$ keV, uncertainties for ENDF/B-VII.1 library, Low-Fidelity project and KADoNiS database [2, 4, 8]. Data are taken from [5].

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III. ^{252}Cf FISSION NEUTRON SPECTRUM AVERAGED CROSS SECTIONS AND THEIR UNCERTAINTIES

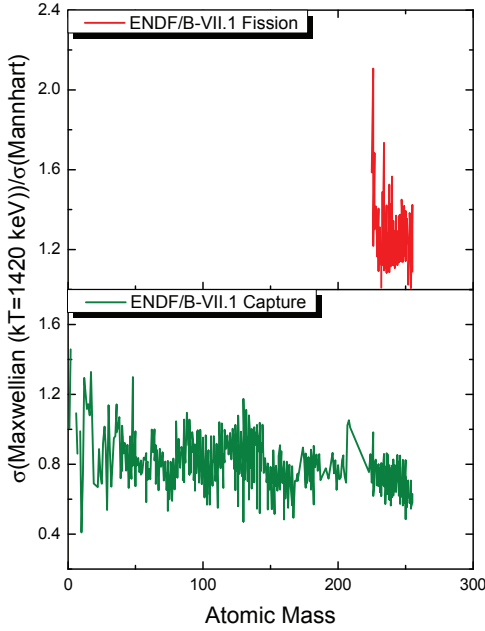


FIG. 2. (Color online) The ratio of calculated ENDF/B-VII.1 californium spectrum neutron cross sections using Maxwellian, $kT=1420$ keV, and Mannhart spectra [5, 10].

^{252}Cf is often used in nuclear physics as a compact, portable and intense neutron source. Its neutron energy spectrum is similar to a fission reactor, with an average energy of 2.13 MeV. This is very convenient for ENDF libraries validation tests in the fast region, even though it is not exactly representative of a fast reactor spectrum (being hotter) [9].

For evaluation purposes, ^{252}Cf spectrum neutron fission and capture averaged cross sections were calculated using Maxwellian-averaged ($kT=1420$ keV) spectrum and Mannhart evaluation [5, 10]. Fig. 2 shows the ratio of calculated californium spectra cross sections using Maxwellian, and Mannhart approaches for ENDF/B-VII.1 library. This ratio indicates that Maxwellian spectrum provides a reasonable fit of californium data, however, it falls short of being used for nuclear standards and dosimetry purposes. Consequently, the Mannhart evaluation has been chosen for calculation of californium spectrum cross sections.

Presently, the original and 640-group representations of Mannhart evaluation are frequently considered. To evaluate a possible spectrum representation impact, neutron cross sections have been calculated using the both formats. Figs. 3, 4 show the ratios of californium fission and capture cross sections for both representations of the linearized ENDF libraries. The plotted ratios clearly demonstrate the impact of different representations.

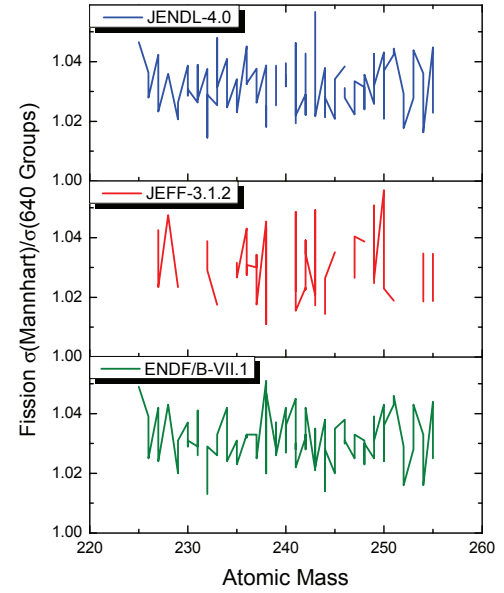


FIG. 3. (Color online) The ratio of ENDF, JEFF, and JENDL calculated californium spectrum neutron fission cross sections using the original and 640-group Mannhart spectra [10].

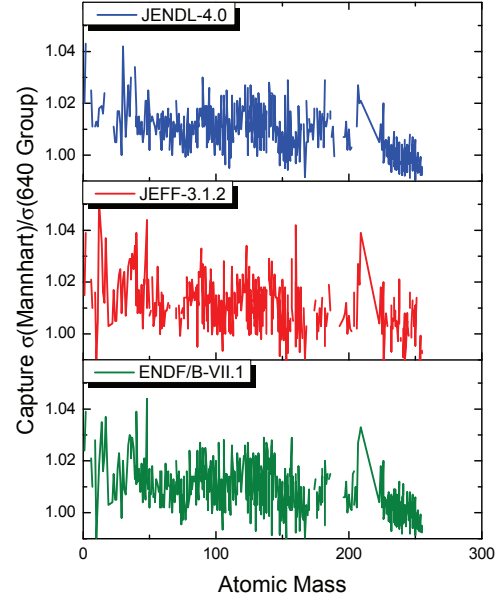


FIG. 4. (Color online) The ratio of ENDF, JEFF, and JENDL calculated californium spectrum neutron capture cross sections using the original and 640-group Mannhart spectra [10].

Following the nuclear dosimetry example, ^{252}Cf spectrum neutron fission averaged cross sections for major evaluated libraries: ENDF/B-VII.1, JEFF-3.1.2, and JENDL-4.0 [2, 11, 12] have been produced using the 640-group format and shown in the Table I. These data are in a good agreement with the previously-published CIELO values [9]. Californium spectrum neutron capture averaged cross sections are available upon request.

TABLE I: 640-group californium spectrum neutron fission averaged cross sections for ENDF, JEFF, and JENDL major evaluated libraries, and EXFOR (experimental nuclear reaction) data ($kT \sim 1.42$ MeV) [2, 11–13].

Material	ENDF/B-VII.1 (barns)	JEFF-3.1.2 (barns)	JENDL-4.0 (barns)	EXFOR (barns)
88-Ra-223	5.485E-2±8.293E-4	5.485E-2±8.293E-4	5.485E-2±8.293E-4	
88-Ra-224				
88-Ra-225				
88-Ra-226	3.741E-4±5.990E-6	3.741E-4±5.990E-6	3.740E-4±5.988E-6	
89-Ac-225	3.505E-2±4.369E-2		3.503E-2±4.379E-2	
89-Ac-226	3.478E-2±4.126E-2		3.472E-2±4.337E-2	
89-Ac-227	1.253E-2±2.089E-3	1.316E-2±1.755E-4	1.252E-2±2.082E-3	
90-Th-227	2.968E-1±2.358E-1	4.747E-1±7.820E-3	2.966E-1±2.402E-1	
90-Th-228	3.768E-1±7.536E-2	1.073E-1±1.443E-3	3.757E-1±7.561E-2	
90-Th-229	3.433E-1±5.660E-2	4.747E-1±7.819E-3	3.431E-1±5.780E-2	
90-Th-230	2.044E-1±1.592E-2		2.042E-1±1.594E-2	
90-Th-231	1.977E-1±1.630E-1		1.977E-1±1.623E-1	
90-Th-232	7.582E-2±1.824E-3		8.170E-2±6.032E-3	8.470E-2±4.900E-3
90-Th-233	9.916E-2±9.237E-2	1.084E-1±1.850E-3	9.918E-2±9.174E-2	
90-Th-234	3.542E-2±4.487E-2		3.541E-2±4.396E-2	
91-Pa-229	1.939E+0±4.916E-1		1.938E+0±4.862E-1	
91-Pa-230	1.782E+0±3.484E-1		1.781E+0±3.463E-1	
91-Pa-231	7.667E-1±1.031E-2	9.843E-1±1.330E-2	8.442E-1±2.385E-2	9.700E-1±4.500E-2
91-Pa-232	9.581E-1±2.711E-1	1.082E+0±1.739E-2	9.572E-1±2.804E-1	
91-Pa-233	2.384E-1±3.065E-3		2.463E-1±5.697E-2	
92-U -230	2.377E+0±5.504E-1		2.375E+0±5.416E-1	
92-U -231	2.162E+0±3.938E-1		2.161E+0±3.900E-1	
92-U -232	2.038E+0±6.916E-2	2.442E+0±3.590E-2	2.038E+0±6.916E-2	
92-U -233	1.867E+0±3.478E-2	1.883E+0±3.130E-2	1.879E+0±2.949E-2	1.947E+0±3.100E-2
92-U -234	1.186E+0±2.199E-1	1.171E+0±1.591E-2	1.211E+0±3.167E-2	
92-U -235	1.209E+0±2.000E-2	1.203E+0±1.913E-2	1.202E+0±2.162E-2	1.266E+0±1.823E-2
92-U -236	5.873E-1±1.371E-1	6.059E-1±7.922E-3	5.801E-1±9.429E-3	
92-U -237	6.320E-1±9.515E-3	8.719E-1±1.339E-2	5.874E-1±8.340E-2	
92-U -238	3.117E-1±4.753E-3	3.102E-1±4.006E-3	3.094E-1±4.815E-3	3.109E-1±1.400E-2
92-U -239	3.730E-1±5.929E-3			
92-U -240	1.953E-1±2.549E-3			
92-U -241	1.881E-1±2.812E-3			
93-Np-234	2.436E+0±4.196E-1		2.436E+0±4.243E-1	
93-Np-235	2.173E+0±5.521E-1	1.878E+0±2.709E-2	2.173E+0±5.495E-1	
93-Np-236	2.062E+0±3.925E-1	1.891E+0±2.975E-2	2.062E+0±3.888E-1	
93-Np-237	1.339E+0±4.624E-2	1.313E+0±1.773E-2	1.322E+0±2.803E-2	1.442E+0±2.300E-2
93-Np-238	1.431E+0±1.659E-1	1.453E+0±2.560E-2	1.430E+0±1.645E-1	
93-Np-239	5.923E-1±5.151E-1		5.916E-1±5.341E-1	
94-Pu-236	2.324E+0±2.389E-1	2.075E+0±3.180E-2	2.324E+0±2.390E-1	
94-Pu-237	2.399E+0±6.080E-1	2.954E+0±4.526E-2	2.400E+0±6.024E-1	
94-Pu-238	1.925E+0±4.890E-2	1.973E+0±2.816E-2	1.944E+0±7.337E-2	
94-Pu-239	1.774E+0±2.865E-2	1.774E+0±2.653E-2	1.777E+0±2.654E-2	1.947E+0±3.100E-2
94-Pu-240	1.334E+0±1.993E-2	1.353E+0±1.822E-2	1.316E+0±1.779E-2	
94-Pu-241	1.579E+0±3.618E-2	1.631E+0±2.579E-2	1.601E+0±3.585E-2	
94-Pu-242	1.140E+0±2.945E-2	1.162E+0±1.560E-2	1.140E+0±2.932E-2	
94-Pu-243	1.062E+0±1.501E-2	1.062E+0±1.501E-2		
94-Pu-244	1.028E+0±2.802E-2		1.029E+0±2.792E-2	
94-Pu-246	5.787E-1±5.108E-1		5.779E-1±5.082E-1	
95-Am-240	1.987E+0±3.776E-1		1.986E+0±3.734E-1	
95-Am-241	1.362E+0±3.067E-2	1.377E+0±1.805E-2	1.385E+0±3.027E-2	
95-Am-242	1.950E+0±3.116E-2	1.726E+0±2.811E-2	1.807E+0±1.844E-1	
95-Am-242M	1.903E+0±3.419E-1	1.813E+0±2.934E-2	1.807E+0±5.952E-2	1.600E+0±2.200E-1
95-Am-243	1.075E+0±1.197E-1	1.077E+0±1.407E-2	1.076E+0±3.698E-2	1.145E+0±2.300E-2
95-Am-244	1.735E+0±2.843E-2	1.735E+0±2.843E-2	1.317E+0±3.417E-1	
95-Am-244M	1.735E+0±2.843E-2	1.735E+0±2.843E-2	1.162E+0±3.674E-1	
96-Cm-240	2.026E+0±4.665E-1	1.719E+0±2.236E-2	2.025E+0±4.587E-1	
96-Cm-241	2.184E+0±5.146E-1	2.639E+0±3.999E-2	2.182E+0±5.178E-1	
96-Cm-242	1.755E+0±2.219E-1	1.643E+0±2.265E-2	1.754E+0±2.272E-1	
96-Cm-243	2.396E+0±8.415E-2	2.137E+0±3.385E-2	2.396E+0±8.418E-2	
96-Cm-244	1.717E+0±7.219E-2	1.591E+0±2.170E-2	1.717E+0±7.195E-2	
96-Cm-245	1.730E+0±7.167E-2	1.711E+0±2.718E-2	1.730E+0±7.159E-2	
96-Cm-246	1.240E+0±7.220E-2	1.217E+0±1.615E-2		
96-Cm-247	1.835E+0±4.952E-2	1.886E+0±2.894E-2	1.835E+0±4.955E-2	
96-Cm-248	1.081E+0±8.008E-2	1.240E+0±1.669E-2	1.081E+0±7.968E-2	
96-Cm-249	1.202E+0±5.710E-1	2.065E+0±3.173E-2	1.202E+0±5.847E-1	
96-Cm-250	6.630E-1±4.282E-1	1.538E+0±1.999E-2	6.630E-1±4.383E-1	
97-Bk-245	1.087E+0±2.234E-1		1.084E+0±2.286E-1	
97-Bk-246	1.732E+0±3.825E-1		1.732E+0±3.889E-1	
97-Bk-247	8.941E-1±3.688E-1	1.014E+0±1.352E-2	8.932E-1±3.681E-1	
97-Bk-248	1.541E+0±3.586E-1		1.541E+0±3.563E-1	
97-Bk-249	1.035E+0±1.564E-1	9.726E-1±1.266E-2	1.033E+0±1.559E-1	
97-Bk-250	1.003E+0±7.197E-1	2.013E+0±3.048E-2	1.003E+0±7.174E-1	
98-Cf-246	2.152E+0±6.765E-1		2.153E+0±6.627E-1	
98-Cf-248	1.323E+0±5.496E-1		1.318E+0±6.115E-1	
98-Cf-249	1.723E+0±6.529E-2	1.723E+0±2.679E-2	1.721E+0±6.506E-2	
98-Cf-250	1.489E+0±8.122E-1	1.877E+0±2.516E-2	1.488E+0±8.109E-1	
98-Cf-251	1.273E+0±4.892E-1	1.696E+0±2.646E-2	1.273E+0±4.870E-1	
98-Cf-252	2.291E+0±1.048E-1	1.897E+0±2.562E-2	2.291E+0±1.047E-1	

TABLE I: 640-group californium spectrum neutron ... (continued).

Material	ENDF/B-VII.1 (barns)	JEFF-3.1.2 (barns)	JENDL-4.0 (barns)	EXFOR (barns)
98-Cf-253	7.674E-1±3.941E-1		7.677E-1±3.918E-1	
98-Cf-254	1.779E+0±6.068E-1	2.133E+0±3.024E-2	1.773E+0±6.573E-1	
99-Es-251	1.355E+0±7.800E-1		1.352E+0±7.677E-1	
99-Es-252	2.143E+0±6.295E-1		2.143E+0±6.307E-1	
99-Es-253	1.028E+0±7.579E-1		1.027E+0±7.546E-1	
99-Es-254	1.901E+0±1.745E-1	2.153E+0±3.260E-2	1.899E+0±1.766E-1	
99-Es-254M	1.885E+0±2.099E-1		1.884E+0±2.076E-1	
99-Es-255	7.059E-1±6.022E-1	2.222E+0±3.150E-2	7.053E-1±5.969E-1	
100-Fm-255	2.189E+0±6.989E-1	2.294E+0±3.473E-2	2.188E+0±7.099E-1	

IV. CROSS SECTION UNCERTAINTIES ANALYSIS AND RECOMMENDATIONS

To evaluate ENDF libraries covariances in the fast neutrons region I will consider Maxwellian, and californium spectra cross sections uncertainties, and deduce recommendations.

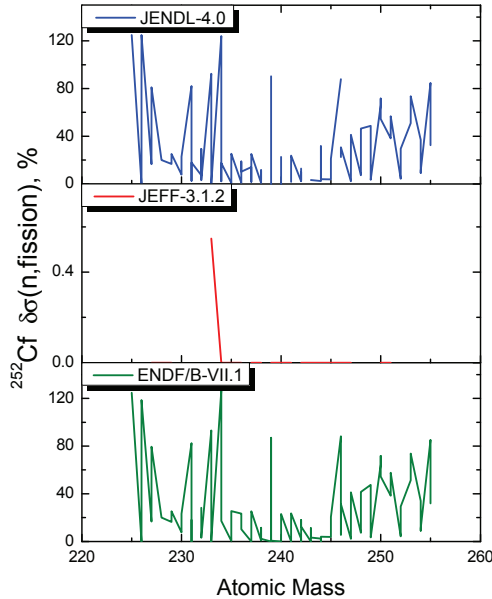


FIG. 5. (Color online) The ENDF, JEFF, and JENDL calculated californium spectrum neutron fission cross section uncertainties using the 640-group Mannhart spectrum [10].

Visual inspection of the shown in Figs. 5, 6 data allows to spot the “suspect” cases, where uncertainties are not very useful for application development. These somewhat unrealistic uncertainties of above 100 and below 1 % originate from theoretical models and fitting procedures, respectively. The summary of re-analysis of the previous Maxwellian data ($kT=30$ keV) [5] and analysis of the current Mannhart spectrum uncertainties for ENDF/B-VII.1 library is shown in the Table II.

The present analysis suggests the following recommendations for ENDF integral values and covariances:

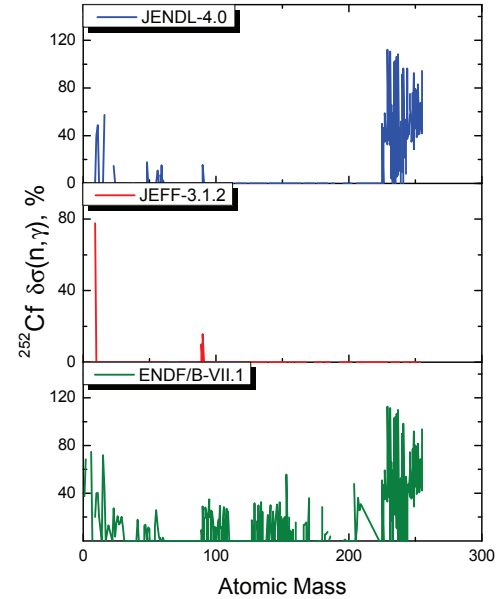


FIG. 6. (Color online) The ENDF, JEFF, and JENDL calculated californium spectrum neutron capture cross section uncertainties using the 640-group Mannhart spectrum [10].

1. Absolute cross section values for linearized files are sensitive to the changes of Mannhart evaluation group structure. Calculated values are model dependent and may vary within 1-5%.
2. Nuclear astrophysics and energy applications require covariances for all ENDF materials.
3. Realistic covariances are needed:
 - Covariance matrices that result in >100 % cross section uncertainties should be avoided, such large uncertainties are not very useful for application development.
 - Covariance matrices that result in <1 % cross section uncertainties are not realistic; strong contradiction with the best experiments.
 - Presently, covariance matrices produce wide variations of cross section uncertainties within 0.5-120 % range. This spread should be kept within 3-50 % range.

TABLE II. The summary of the ENDF/B-VII.1 library cross section uncertainties analysis.

Reaction	Maxwellian spectrum, $kT=30$ keV		Mannhart spectrum [10]	
	Uncertainty <1%	Uncertainty >100%	Uncertainty <1%	Uncertainty >100%
(n,fission)	^{235}U , $^{239,240}\text{Pu}$	$^{225,226}\text{Ac}$, ^{233}Th , ^{229}Pa , ^{235}Np , ^{246}Pu , ^{250}Cm , $^{247,250}\text{Bk}$, $^{246,248,250,254}\text{Cf}$, $^{251,253,255}\text{Es}$	$^{235,238}\text{U}$, $^{239,240}\text{Pu}$	$^{225,226}\text{Ac}$, ^{234}Th
(n, γ)		^{229}Pa , ^{237}Pu , ^{249}Cm , ^{250}Bk , ^{255}Fm	^{52}Cr	^{229}Pa , ^{231}U , $^{234,235,236}\text{Np}$, ^{237}Pu

4. Multiple MF=33 covariance matrices can be confusing.

V. CONCLUSIONS

The previously-calculated ENDF/B-VII.1 and Low-Fidelity Maxwellian-averaged cross section uncertainties have been re-analyzed. Californium spectrum neutron fission and capture averaged cross sections and their uncertainties have been calculated for ENDF/B-VII.1,

JEFF-3.1.2, and JENDL-4.0 nuclear data libraries. Recommendations for ENDF covariances have been deduced using the application development needs.

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